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Book of Abstracts

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CHARGE AND ORBITAL ORDER IN SODIUM COBALTATES Na_xCoO_2

Mukhamedshin I.R.[1,2], *Alloul H.*[2]
[1] Institute of Physics, Kazan Federal University, 420008, Kazan, Russia
[2] Laboratoire de Physique des Solides, Université Paris-Sud, 91405, Orsay, France
Irek.Mukhamedshin@kpfu.ru

The influence of the dopant atoms on the electronic properties of conducting layers has initiated large debates in high temperature superconducting cuprates as well as in other complex layered oxides of transition elements. Whereas in many systems this influence is masked by miscellaneous effects, there are many experimental evidences that in the sodium cobaltates Na_xCoO_2 a large interplay between the Na atomic ordering and the electronic density on the Co sites occurs. The Na_1CoO_2 phase is a band insulator in which the Co sites are in filled-shell nonmagnetic Co^{3+} states. At x<1 the system becomes metallic, but only specific Na compositions can be obtained, which correspond to some Na orderings as observed by diffraction techniques. E.g. for x=0.5 the Na atoms are ordered in an orthorhombic superstructure commensurate with the Co lattice and a small charge disproportionation into $Co^{3.5\pm\varepsilon}$ (with ε<0.2) occurs on the two Co sites .

We have synthesized and characterized different stable phases of sodium cobaltates Na_xCoO_2 with sodium content 0.65<x<0.80, including one of the most stable magnetic phases of sodium cobaltates with a well defined Néel temperature of T_N=22 K. We demonstrate that ^{23}Na NMR allows to determine the difference in the susceptibility of the phases and reveals the presence of Na order in each phase. Our detailed NMR /NQR studies allowed us to reveal the peculiarities of the x=2/3 phase. We could establish reliably the atomic order of the Na layers and their stacking between the CoO_2 slabs. We found that the Na^+ order stabilizes filled non magnetic Co^{3+} ions on 25% of the cobalt sites Co1 arranged in a triangular sublattice. The transferred holes are delocalized on the 75% complementary cobalt sites Co2 which unexpectedly display a planar cobalt kagomé structure [2].

^{59}Co NMR experiments give clear evidence that such Co charge disproportionation is a dominant feature of Na cobaltates for 0.65<x<0.80 [3]. Only a small fraction (≈25%) of cobalts are in a non-magnetic Co^{3+} charge state whereas electrons delocalize on the other cobalts. We found that the magnetic and charge properties of the Co sites are highly correlated with each other as magnetic shift K_{ZZ} scale linearly with quadrupolar frequency ν_Q [2]. Such correlations can be understood as both measured values ν_Q and K_{ZZ} contain terms proportional to the quadrupole moment of the t_{2g} hole density distribution which involves as a coefficient the hole concentration on the Co site. Therefore this correlations reflects the fact that the hole contenton the Co orbitals varies from site to site in both phases and the hyperfine coupling (or the local magnetic susceptibility) scales with the on site delocalized charge. Such unusual charge differentiation in sodium cobaltates calls for better theoretical understanding of the incidence of the Na atomic order on the electronic structures of these compounds.

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